

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,  
AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.

NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 13:55:56 ON 23 FEB 2010

=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE  
ENTRY  
SESSION  
TOTAL  
0.22  
0.22

FILE 'REGISTRY' ENTERED AT 13:56:16 ON 23 FEB 2010  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2  
DICTIONARY FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2

New CAS Information Use Policies: enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stnqgen/stndoc/properties.html>

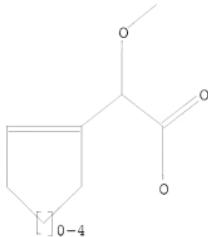
=>  
Uploading c:\documents and settings\pzucker\my documents\examination auxillary  
file\10566995\10566995.amdt.11.23.09.mpg.cmds

## 1.1 STRUCTURE UPLOADED

→ d. 11

→ **Q 11**  
LJ HAS NO ANSWERS

IT HAS NO ANSWERS



Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam

SAMPLE SEARCH INITIATED 13:56:56 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 12484 TO ITERATE

16.0% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 242984 TO 256376  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search 11 sss full

FULL SEARCH INITIATED 13:57:13 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 251170 TO ITERATE

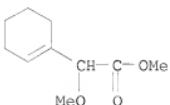
100.0% PROCESSED 251170 ITERATIONS  
SEARCH TIME: 00.00.01

31 ANSWERS

L3 31 SEA SSS FUL L1

=> d scan

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -methoxy-, methyl ester  
MF C10 H16 O3

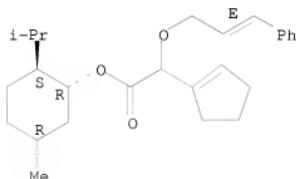


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):32

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -[(2E)-3-phenyl-2-propen-1-yl]oxy]-,  
(1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester  
MF C26 H36 O3

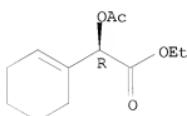
Absolute stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(acetyloxy)-, ethyl ester, (R)- (9CI)  
MF C12 H18 O4

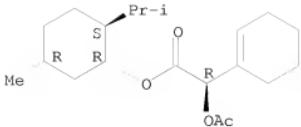
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

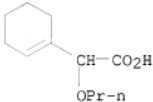
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(acetyloxy)-,  
5-methyl-2-(1-methylethyl)cyclohexyl ester,  
[1R-[1a(R\*),2B,5a]]- (9CI)  
MF C20 H32 O4

Absolute stereochemistry.



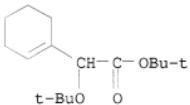
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -propoxy-  
 MF C11 H18 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

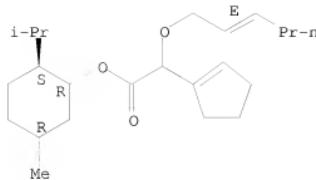
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(1,1-dimethylethoxy)-,  
 1,1-dimethylethyl ester  
 MF C16 H28 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -(2E)-2-hexen-1-yloxy)-,  
 (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester  
 MF C23 H38 O3

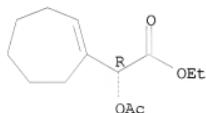
Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cycloheptene-1-acetic acid,  $\alpha$ -(acetoxy)-, ethyl ester, (R)-  
 (9CI)  
 MF C13 H20 O4

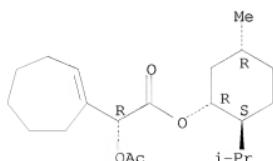
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

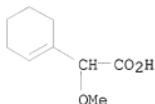
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cycloheptene-1-acetic acid,  $\alpha$ -(acetoxy)-,  
 5-methyl-2-(1-methylethyl)cyclohexyl ester,  
 [1R-[1a(R\*),2B,5a]]- (9CI)  
 MF C21 H34 O4

Absolute stereochemistry.



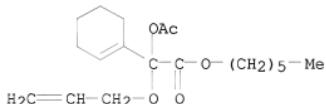
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -methoxy-  
MF C9 H14 O3  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

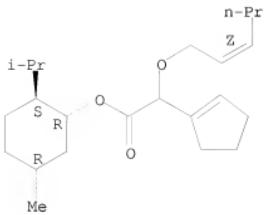
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(acetyloxy)- $\alpha$ -(2-propen-1-yloxy)-, hexyl ester  
MF C19 H30 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -[(2Z)-2-hexen-1-yloxy]-,  
(1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester  
MF C23 H38 O3

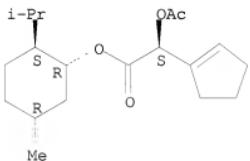
Absolute stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

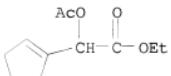
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -(acetoxy)-,  
 5-methyl-2-(1-methylethyl)cyclohexyl ester,  
 [1R-[1a(S\*),2 $\beta$ ,5a]]- (9CI)  
 MF C19 H30 O4

Absolute stereochemistry.



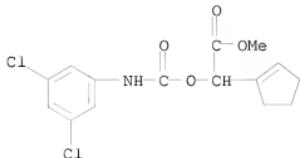
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -(acetoxy)-, ethyl ester  
 MF C11 H16 O4



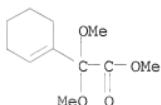
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -[(3,5-dichlorophenyl)amino]carbonyl]oxy]-, methyl ester  
MF C15 H15 Cl2 N O4



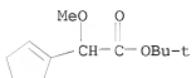
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha,\alpha$ -dimethoxy-, methyl ester  
MF C11 H18 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -methoxy-, 1,1-dimethylethyl ester  
MF C12 H20 O3

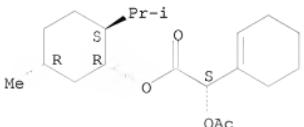


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

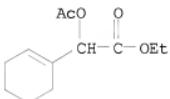
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(acetyloxy)-,  
5-methyl-2-(1-methylethyl)cyclohexyl ester,  
[1R-[1a(S\*)<sup>2</sup>,2 $\beta$ ,5 $\alpha$ ]- (9CI)  
MF C20 H32 O4

Absolute stereochemistry.



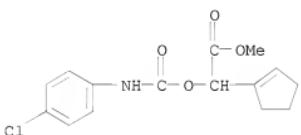
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(acetyloxy)-, ethyl ester  
MF C12 H18 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

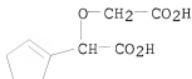
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -[[(4-  
chlorophenyl)amino]carbonyl]oxy]-, methyl ester  
MF C15 H16 Cl N O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

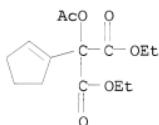
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -(carboxymethoxy)-  
MF C9 H12 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

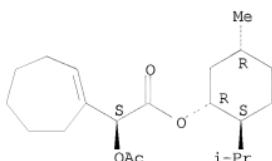
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN Propanedioic acid, 2-(acetoxy)-2-(1-cyclopenten-1-yl)-, 1,3-diethyl  
ester  
MF C14 H20 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

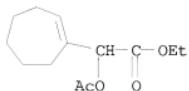
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cycloheptene-1-acetic acid,  $\alpha$ -(acetoxy)-,  
5-methyl-2-(1-methylethyl)cyclohexyl ester,  
[1R-[1a(S'),2 $\beta$ ,5a]]- (9CI)  
MF C21 H34 O4

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

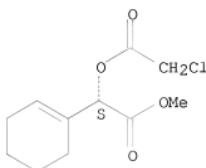
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cycloheptene-1-acetic acid,  $\alpha$ -(acetoxy)-, ethyl ester  
MF C13 H20 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

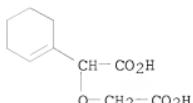
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -[(chloroacetyl)oxy]-, methyl ester,  
(S)- (9CI)  
MF C11 H15 Cl O4

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

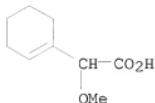
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(carboxymethoxy)-  
MF C10 H14 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -methoxy-, compd. with phenylmethyl carbamimidothioate (1:1)  
MF C9 H14 O3 . C8 H10 N2 S

CM 1

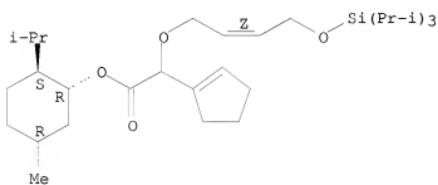


CM 2



L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -[(2Z)-4-[(tris(1-methylethyl)silyl)oxy]-2-buten-1-yl]oxy]-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester  
MF C30 H54 O4 Si

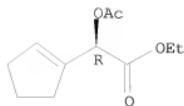
Absolute stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -(acetyloxy)-, ethyl ester, (R)- (9CI)  
MF C11 H16 O4

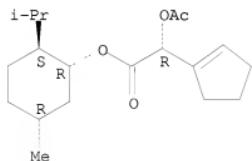
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

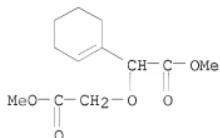
L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclopentene-1-acetic acid,  $\alpha$ -(acetoxy)-,  
 5-methyl-2-(1-methylethyl)cyclohexyl ester,  
 [1R-[1a(R\*),2 $\beta$ ,5 $\alpha$ ]]- (9CI)  
 MF C19 H30 O4

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 31 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 1-Cyclohexene-1-acetic acid,  $\alpha$ -(2-methoxy-2-oxoethoxy)-, methyl  
 ester  
 MF C12 H18 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> e 1-Cyclopentene-1-acetic acid,  $\alpha$ -methoxy-, 1,1-dimethylethyl ester/cn  
L4 0 E1-CYCLOPENTENE-1-ACETIC ACID, A-METHOXY-, 1,1-DIMETHYLETHYL  
ESTER/CN

=> e 1-Cyclopentene-1-acetic acid,  $\alpha$ -methoxy-, 1,1-dimethylethyl ester/cn  
E1 1 1-CYCLOPENTENE-1-ACETIC ACID, TERT-BUTYL ESTER/CN  
E2 1 1-CYCLOPENTENE-1-ACETIC ACID, TRIMETHYLSILYL ESTER/CN  
E3 0 --> 1-CYCLOPENTENE-1-ACETIC ACID, A-METHOXY-, 1,1-DIMETHYLETHYL  
ESTER/CN  
E4 1 1-CYCLOPENTENE-1-ACETIC-CARBOXY-14C ACID, 3-CARBOXY-, DIETHYL  
ESTER/CN  
E5 1 1-CYCLOPENTENE-1-ACETO-2',5'-XYLIDIDE/CN  
E6 1 1-CYCLOPENTENE-1-ACETO-O-TOLUIDIDE/CN  
E7 1 1-CYCLOPENTENE-1-ACETO-P-TOLUIDIDE/CN  
E8 1 1-CYCLOPENTENE-1-ACETONITRILE/CN  
E9 1 1-CYCLOPENTENE-1-ACETONITRILE, A,A-DIMETHYL-3-OX  
O/CN  
E10 1 1-CYCLOPENTENE-1-ACETONITRILE, A,2,4,4-TETRAMETHYL-5-O  
XO/CN  
E11 1 1-CYCLOPENTENE-1-ACETONITRILE, A-(((1-METHYLETHYL)SUL  
FONYL)(OXY)IMINO)-/CN  
E12 1 1-CYCLOPENTENE-1-ACETONITRILE, A-(((3,3,3-TRIFLUOROPRO  
PYL)SULFONYL)METHYL)-/CN

=> e 1-Cyclopentene-1-acetic acid,  $\alpha$ -methoxy-, 1,1-dimethylethyl ester/cn  
E1 1 1-CYCLOPENTENE-1-ACETANILIDE, N,2,3,3-TETRAMETHYL-/CN  
E2 1 1-CYCLOPENTENE-1-ACETIC ACID/CN  
E3 0 --> 1-CYCLOPENTENE-1-ACETIC ACID, A-METHOXY-, 1,1-DIMETHYL  
ETHYL ESTER/CN  
E4 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A,2-TRIMETHYL-,  
ET ESTER/CN  
E5 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A,2-TRIMETHYL-,  
ETHYL ESTER/CN  
E6 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A-DIFLUORO-, ETH  
YL ESTER/CN  
E7 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A-DIMETHYL-/CN  
E8 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A-DIMETHYL-, ETH  
YL ESTER/CN  
E9 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A-DIMETHYL-, MET  
HYL ESTER/CN  
E10 1 1-CYCLOPENTENE-1-ACETIC ACID, A,A-DIMETHYL-5-PHE  
NYL-, METHYL ESTER/CN  
E11 1 1-CYCLOPENTENE-1-ACETIC ACID, A,2-DIMETHYL-5-OXO-, (5-  
(2-THIENYLMETHYL)-3-FURANYL)METHYL ESTER/CN  
E12 1 1-CYCLOPENTENE-1-ACETIC ACID, A,3,3,5-TETRAMETHYL-, ET  
HYL ESTER/CN

=> e 1-Cyclopentene-1-acetic acid,  $\alpha$ -methoxy-, 1,1-dimethylethyl ester/cn  
E1 1 1-CYCLOPENTENE-1-ACETIC ACID, A-ISOCYANO-A-METHY  
L-, METHYL ESTER/CN  
E2 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHOXY-, 1,1-DIMETHYL  
ETHYL ESTER/CN  
E3 0 --> 1-CYCLOPENTENE-1-ACETIC ACID, A-METHOXY-, 1,1-DIMETHYLE  
THYL ESTER/CN  
E4 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-/CN  
E5 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-, (5-(PHENYLMET  
HYL)-3-FURANYL)METHYL ESTER/CN  
E6 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-, 1,1-DIMETHYLE

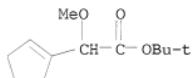
THYL ESTER/CN  
 E7 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-, ETHYL ESTER/C  
 N  
 E8 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-, METHYL ESTER/CN  
 E9 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-A-((3,3,  
 3-TRIFLUOROPROPYL)SULFONYL)METHYL)-, METHYL ESTER/CN  
 E10 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-A-((3,3,  
 3-TRIFLUOROPROPYL)SULFONYL)-, METHYL ESTER/CN  
 E11 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-A-(PHENYL  
 THIO)-, METHYL ESTER/CN  
 E12 1 1-CYCLOPENTENE-1-ACETIC ACID, A-METHYL-2-((4-METHYL-3-  
 FURANYL)METHYL)-3-(PHENYLMETHOXY)-/CN

=> e2

L5 1 "1-CYCLOPENTENE-1-ACETIC ACID, A-METHOXY-, 1,1-DIMETHYLETHYL ESTER"/CN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN  
 RN 286455-99-0 REGISTRY  
 ED Entered STN: 18 Aug 2000  
 CN 1-Cyclopentene-1-acetic acid,  $\alpha$ -methoxy-, 1,1-dimethylethyl  
 ester (CA INDEX NAME)  
 MF C12 H20 O3  
 SR CA  
 LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 15  
L6 1 L5  
=> d 16 ti fbib abs

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN  
TI Regiochemistry of molybdenum-catalyzed O-H insertions of vinylcarbenoids  
AN 2000:443464 CAPLUS <>LOGINID::20100223>>  
DN 133:176928  
TI Regiochemistry of molybdenum-catalyzed O-H insertions of vinylcarbenoids  
AU Davies, H. M. L.; Yokota, Y.  
CS Department of Chemistry, State University of New York at Buffalo, Buffalo,  
NY, 14260-3000, USA  
SO Tetrahedron Letters (2000), 41(25), 4851-4854  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
AB Molybdenum-catalyzed decomposition of vinyldiazoacetates generates  
vinylcarbenoids that preferentially react with alcs. at the vinylous  
position of the vinylcarbenoid rather than at the carbene site.  
OSC.G 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)  
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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DICTIONARY FILE UPDATES: 21 FEB 2010 HIGHEST RN 1206966-88-2

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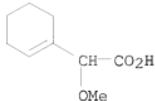
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=> E 1-Cyclohexene-1-acetic acid,  $\alpha$ -methoxy-/CN  
E1 1 1-CYCLOHEXENE-1-ACETIC ACID, A-HYDROXY-6-OXO-, (1R,2S,  
5R)-5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ESTER, (AS)-/  
CN  
E2 1 1-CYCLOHEXENE-1-ACETIC ACID, A-ISOCYANO-A-METHYL  
-, METHYL ESTER/CN  
E3 1 --> 1-CYCLOHEXENE-1-ACETIC ACID, A-METHOXY-/CN  
E4 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHOXY-, COMPD. WITH P  
HENYLMETHYL CARBAMIMIDOTHIOATE (1:1)/CN  
E5 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHOXY-, METHYL ESTER/  
CN  
E6 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-/CN  
E7 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-, (5-(PHENYLMETH  
YL)-3-FURANYL)METHYL ESTER/CN  
E8 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-, (S)-/CN  
E9 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-, 1,1-DIMETHYLET  
HYL ESTER/CN  
E10 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-, 2-(DIETHYLAMIN  
O)ETHYL ESTER/CN  
E11 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-, 2-DIETHYLAMINO  
ETHYL ESTER/CN  
E12 1 1-CYCLOHEXENE-1-ACETIC ACID, A-METHYL-, 2-HYDROXY-.ALP  
HA.-METHYLCYCLOHEXANEACETIC ACID  $\Gamma$ -LACTONE/CN  
  
=> E3  
L7 1 "1-CYCLOHEXENE-1-ACETIC ACID, A-METHOXY-"/CN  
  
=> D L7

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN  
RN 105105-90-6 REGISTRY  
ED Entered STN: 08 Nov 1986  
CN 1-Cyclohexene-1-acetic acid,  $\alpha$ -methoxy- (CA INDEX NAME)  
MF C9 H14 O3  
CI COM  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)



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2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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| FULL ESTIMATED COST                        | 8.09       | 236.45  |  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |  |
|  | ENTRY      | SESSION |  |
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=> L7  
 L8                    2 L7

=> D L8 1-2 TI FBIB ABS

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN  
TI Cyclohexene-1-carboxaldehyde  
AN 1959:34474 CAPLUS <<LOGINID::20100223>>  
DN 53:34474  
OREF 53:6110d-h  
TI Cyclohexene-1-carboxaldehyde  
AU Bergmann, Ernst D.; Becker, Abraham  
CS Hebrew Univ., Jerusalem, Israel  
SO Journal of Organic Chemistry (1958), 23, 1553-4  
CODEN: JOCEAH; ISSN: 0022-3263  
DT Journal  
LA Unavailable  
OS CASREACT 53:34474  
AB Cyclohexenyltrichloromethylcarbinol (I) heated with 4 moles of 20% NaOH gave 25% cyclohexenylglycolic acid (II), but the yield of cyclohexene-1-carboxaldehyde (III) was more variable, much polymeric material being formed. All expts. failed to pyrolyze I in the presence of KOH, K<sub>2</sub>CO<sub>3</sub>, or Cu powder, or to split it by means of concentrated H<sub>2</sub>SO<sub>4</sub> or Pb(OAc)<sub>4</sub>. I (82%) was prepared from 1 mole Cl<sub>3</sub>CCHO, 2 moles cyclohexene, and 14 g. AlCl<sub>3</sub>, b15 150°. I (1 mole) and 2 moles NaOMe in 500 ml. MeOH refluxed 3 hrs., the alc. removed, the solid filtered off, washed, and the filtrate and washings treated with H<sub>2</sub>O and 200 ml. Et<sub>2</sub>O, the ethereal layer dried, and distilled gave 90% dicyclohexenyl glycolide (IV), b20 140°. I (57 g.) and 50 g. NaOH in 100 ml. H<sub>2</sub>O refluxed 1 hr., cooled, extracted with Et<sub>2</sub>O, and acidified gave 10 g. II, b30 155°, m. 125°. IV (27.6 g.) refluxed 3 hrs. with 8 g. NaOH in 100 ml. H<sub>2</sub>O yielded 30 g. I, which solidified spontaneously and m. 125° without further purification. Treatment of I with 5 moles NaOH in MeOH or PrOH gave cyclohexenylmethoxy-acetic acid (V), b0.1 124°, and cyclohexenylpropoxy-acetic acid (VI), b25 156°, resp. Pyrolysis of V and VI with Cu powder gave 54 and 73% III, so that the over-all yield, calculated on cyclohexene, was 15 and 49%, resp. NaOH (50 g.) in 200 ml. MeOH mixed with 57 g. I and the mixture refluxed 1 hr. after the exothermic reaction subsided, the alc. removed, H<sub>2</sub>O added, and the mixture extracted with Et<sub>2</sub>O and the aqueous layer acidified gave 23 g. V. The same result was obtained when NaOMe was used instead of NaOH. IV (27.6 g.), 18 g. NaOMe, and 100 ml. alc. refluxed 2 hrs., H<sub>2</sub>O added, and the mixture acidified gave 31 g. V. NaOH (50 g.) in 300 ml. PrOH refluxed 1 hr. with 57 g. I gave 36 g. VI, b25 156°. V (17 g.) and 1 g. Cu powder heated 2 hrs. at 200° gave 3.7 g. III, b1 61°. Similarly, 10 g. VI and 1 g. Cu powder heated 2 hrs. at 200° gave 4.5 g. III; 2,4-dinitrophenylhydrazone, m. 212° (BuOH).

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN  
TI Olefinic acid. VIII.  $\alpha$ -Bromocyclohexylideneacetic acid  
AN 1954:3364 CAPLUS <<LOGINID::20100223>>  
DN 48:3364  
OREF 48:574c-i,575a-b  
TI Olefinic acid. VIII.  $\alpha$ -Bromocyclohexylideneacetic acid  
AU Newman, D. D. E.; Owen, L. N.  
CS Imperial Coll. Sci. Technol., London  
SO Journal of the Chemical Society (1952) 4713-21  
CODEN: JCSOA9; ISSN: 0368-1769  
DT Journal  
LA Unavailable  
OS CASREACT 48:3364  
AB cf. C.A. 44, 4863i. Cyclohexylideneacetic acid (I), m. 90-1°, has a maximum absorption at 2260A. (ε 13,200). In the presence of BF<sub>3</sub>, cyclohexanone and CH<sub>2</sub>CO react to give 1-cyclohexeneacetic acid, m. 36-7°; 1,2-dibromide, m. 119-20°. Br (15.9 g.) in 30 cc. HOAc was added over 1 hr. to 13.5 g. I in 80 cc. HOAc at 15°.

After removal of HOAc and recrystn. of the solid product from light petr. gave 1,α-dibromocyclohexaneacetic acid (II), m. 136-7°. II (2.0 g.), shaken with 200 cc. 0.12N NaOH for 1 hr., extracted with ether, the exts. dried and distilled, gave 0.88 g. α-bromomethylenecyclohexane (III), b15 75-6°, n19D 1.5165, also obtained by heating I with pyridine for 1 hr. at 60-5°. Oxidation of III with KMnO4 gave cyclohexanone. An ice cold solution of NaOBt (2.15 g. Na and 30 cc. absolute EtOH) was added to a solution of 12.5 g. II in 50 cc. absolute EtOH at -15°, the solution warmed to room temperature in 16 hrs., the alc. removed, and the residue acidified, gave 7.8 g. α-bromocyclohexylideneacetic acid (IV), m. 120°;  $\lambda$ EtOHmax.: 2260, 2420, 2470, 2510A.; p-bromophenacyl ester, m. 113°. A mixture of 0.99 g. IV and 10 cc. 5N NaOMe-MeOH boiled for 24 hrs. gave α-methoxy-1-cyclohexeneacetic acid (V), m. 59-60°,  $\lambda$ EtOHmax. 2260A.; Me ester, b16 125°, b0.5 90°, n15D 1.4712; S-benzylthiuronium salt m. 179°. Reaction rate data for the formation of V from IV indicates a rearrangement to α-bromo-1-cyclohexeneacetic acid (VII) precedes methanolysis. Acidification of the residue from the isolation V gave, on filtration, the double salt (C8H13O)CO2H.(C8H13O)CO2Na, m. 201-2°. Evaporation of the filtrate gave an oil which, with CH2N2, gave what is probably a mixture of VI and Me α-methoxycyclohexylideneacetate. Heating 4.5 g. IV 24 hrs. with 45 cc. 5N MeONa-MeOH gave, on dilute with water, extraction with Et2O, and acidification of the aqueous solns., 2-hydroxy-α-methoxycyclohexaneacetic acid lactone (VIII), b30 120°, n16D 1.4710, and V. A solution of 2.17 g. V in 20 cc. CC14, ozonized at 0°, and steam distilled after decomposition at 100° with 2N H2SO4, gave methoxymethyl cyclopentyl ketone; semicarbazone, m. 192-3°. Oxidation of V with KMnO4 gave adipic acid. Hydrogenation of V at pH 9 over Pd-C catalyst in H2O gave α-methoxycyclohexaneacetic acid (IX), m. 67°. Et cyclohexaneacetate (X), b0.2 42-3°, n15D 1.4470, prepared by reduction of PhCH2CO2Et, gave cyclohexaneacetic acid, b0.3 75°, m. 26-7°. α-Hydroxycyclohexaneacetic acid (XI) (5.7 g.), m. 135°, was obtained by treating 12.5 g. Et α-bromocyclohexaneacetate (XII) (b0.4 86-7°) with 100 cc. 2.5N NaOH and 50 cc. dioxane for 16 hrs. on a steam bath. XI (2.05 g.), 12 g. Ag2O, and 20 g. MeI shaken together, heated at 65° for 2 hrs., extracted with Et2O, the exts. evaporated, C6H6 added, water removed by azeotropic distillation, and the residue remethylated gave 1.48 g. Me α-methoxycyclohexaneacetate (XIII), b30 120°, n16D 1.4520; hydrolysis gave IX; p-bromophenacyl ester, m. 70°. XII (6.4 g.) heated for 16 hrs. with 50 cc. 2N MeONa-MeOH, poured into H2O, extracted with Et2O, and the dried exts. distilled, gave IX. IX (1.3 g.) neutralized with 2N NaOH, 0.87 g. KMnO4 in 50 cc. H2O added slowly at -15°, and warmed to room temperature, gave 0.30 g. α-oxocyclohexaneacetic acid (XIV), b10 98°, m. 45-9°; 2,4-dinitrophenylhydrazone, m. 211-12°. V does not isomerize in 48 hrs. with 5N MeONa-MeOH at 100°. IV gave polymeric products when heated with 2N NaOH 2.5 days at 125°. 2-Methoxycyclohexanone (XV) (b15 76°, n20D 1.4535) was prepared by methylation of 2-hydroxycyclohexanone; semicarbazone of XV, m. 178-9°. XV reacts with 2,4-dinitrophenylhydrazine to give 1,2-cyclohexandione bis(2,4-dinitrophenylhydrazone), m. 220-1°, and XV 2,4-dinitrophenylhydrazone, m. 135°. XV (4.43 g.), 2.26 g. activated Zn, 5.8 g. BrCH2CO2Et, 14 cc. C6H6, and 12 cc. MePh were heated on a steam bath (vigorous reaction) until the Zn dissolved, filtered, the filtrate decomposed with ice cold 2N HCl; the organic layer, separated, washed with saturated NaHCO3 until neutral, and distilled, gave Et 1-hydroxy-2-methoxycyclohexaneacetate (XVI), b0.5 79-82°, n20D 1.4590; hydrolysis gave impure acid (XVII), n14D 1.4736. XVII dehydrated with Ac2O gave a mixture (XVIII) (n35D 1.4945) of the lactones of

2-hydroxycyclohexylideneacetic acid (XIX) (25%) (m. 21-4°) and  
2-hydroxy-1-cyclohexeneacetic acid (75%). XVIII dissolved in 2N NaOH,  
warmed for 10 min., diluted with water, and extracted with ether, and the  
aqueous  
solution acidified, gave XIX and impure 2-oxocyclohexaneacetic acid;  
2,4-dinitrophenylhydrazone, m. 191-3°; semicarbazone, m.  
192-3°.

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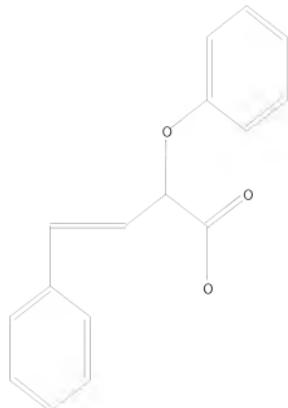
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L9 STRUCTURE UPLOADED

=> D L9  
L9 HAS NO ANSWERS  
L9 STR



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=> SEARCH L9 SSS SAM  
 SAMPLE SEARCH INITIATED 14:26:51 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 101 TO ITERATE

100.0% PROCESSED 101 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 1418 TO 2622  
 PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=> SEARCH L9 SSS FULL  
 FULL SEARCH INITIATED 14:27:00 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 2054 TO ITERATE

100.0% PROCESSED 2054 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

L11 0 SEA SSS FUL L9

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 FULL ESTIMATED COST 192.03 438.18  
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 ENTRY SESSION  
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| NEWS 5  | AUG 24 CA/Cplus enhanced with legal status information for U.S. patents  |
| NEWS 6  | SEP 09 50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY   |
| NEWS 7  | SEP 11 WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus   |
| NEWS 8  | OCT 21 Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded                                 |
| NEWS 9  | OCT 21 Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models |
| NEWS 10 | NOV 23 Addition of SCAN format to selected STN databases   |
| NEWS 11 | NOV 23 Annual Reload of IFI Databases  |
| NEWS 12 | DEC 01 FRFULL Content and Search Enhancements  |
| NEWS 13 | DEC 01 DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets                         |
| NEWS 14 | DEC 02 Derwent World Patent Index: Japanese FI-TERM thesaurus added  |
| NEWS 15 | DEC 02 PCTGEN enhanced with patent family and legal status display data from INPADOCDB                               |
| NEWS 16 | DEC 02 USGENE: Enhanced coverage of bibliographic and sequence information   |
| NEWS 17 | DEC 21 New Indicator Identifies Multiple Basic Patent Records Containing Equivalent Chemical Indexing in CA/Cplus    |
| NEWS 18 | JAN 12 Match STN Content and Features to Your Information Needs, Quickly and Conveniently                            |
| NEWS 19 | JAN 25 Annual Reload of MEDLINE database   |
| NEWS 20 | FEB 16 STN Express Maintenance Release, Version 8.4.2, Is Now Available for Download                                 |
| NEWS 21 | FEB 16 Derwent World Patents Index (DWPI) Revises Indexing of Author Abstracts                                       |
| NEWS 22 | FEB 16 New FASTA Display Formats Added to USGENE and PCTGEN  |
| NEWS 23 | FEB 16 INPADOCDB and INPAFAMDB Enriched with New Content and Features  |
| NEWS 24 | FEB 16 INSPEC Adding Its Own IPC codes and Author's E-mail   |

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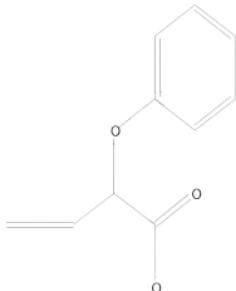
=> Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10566995\10566995 coire.str

L1 STRUCTURE UPLOADED

=> d 11

## L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam  
SAMPLE SEARCH INITIATED 08:01:54 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1512 TO ITERATE

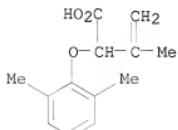
100.0% PROCESSED 1512 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 27908 TO 32572  
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> d scan

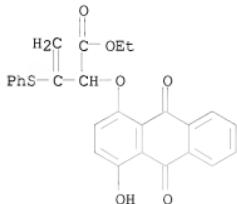
L2 2 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-(2,6-dimethylphenoxy)-3-methyl-  
MF C13 H16 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 2 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-[(9,10-dihydro-4-hydroxy-9,10-dioxo-1-anthracenyl)oxy]-  
3-(phenylthio)-, ethyl ester  
MF C26 H20 O6 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> e 3-Butenoic acid, 2-(2,6-dimethylphenoxy)-3-methyl-/cn  
E1 1 3-BUTENOIC ACID, 2-(2,5-DIMETHOXYPHENYL)-2-OXOETHYL ESTER/CN  
E2 1 3-BUTENOIC ACID, 2-(2,6-DICHLOROPHENYL)HYDRAZIDE/CN  
E3 1 --> 3-BUTENOIC ACID, 2-(2,6-DIMETHYLPHENOXY)-3-METHYL-/CN  
E4 1 3-BUTENOIC ACID, 2-(2,6-DIMETHYLPHENOXY)-3-METHYL-, METHYL E  
STER/CN  
E5 1 3-BUTENOIC ACID, 2-(2,6-DIMETHYLPHENYL)HYDRAZIDE/CN  
E6 1 3-BUTENOIC ACID, 2-(2,6-XYLYL)HYDRAZIDE/CN  
E7 1 3-BUTENOIC ACID, 2-(2-((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY  
)ETHYL)-3-METHYL-, ETHYL ESTER/CN  
E8 1 3-BUTENOIC ACID, 2-(2-((1,1-DIMETHYLETHYL)DIPHENYLSILYL)OXY  
)ETHYLIDENE)-4-(4-((5-((3AS,4S,6AR)-HEXAHYDRO-2-OXO-1H-THIEN  
O(3,4-D)IMIDAZOL-4-YL)-1-OXOPENTYL)AMINO)PHENYL)-, 2-(2-(((7  
(-DIETHYLAMINO)-2-OX/CN  
E9 1 3-BUTENOIC ACID, 2-(2-((1,1-DIMETHYLETHYL)DIPHENYLSILYL)OXY  
)ETHYLIDENE)-4-(4-((6-((7-NITRO-2,1,3-BENZOXADIAZOL-4-YL)AMI  
NO)-1-OXOHEXYL)AMINO)PHENYL)-, 2-(2-((7-(DIETHYLAMINO)-2-OX  
O-2H-1-BENZOPYRAN-3-/CN  
E10 1 3-BUTENOIC ACID, 2-(2-((1,1-DIMETHYLETHYL)DIPHENYLSILYL)OXY  
)ETHYLIDENE)-4-PHENYL-, 2-(2-((7-(DIETHYLAMINO)-2-OXO-2H-1-  
BENZOPYRAN-3-YL)CARBONYL)AMINO)ETHOXO)ETHYL ESTER, (2E,3E)-/ CN  
E11 1 3-BUTENOIC ACID, 2-(2-((2-((2-((AMINOIMINOMETHYL)AMINO)-4-  
THIAZOLYL)METHYL)THIO)ETHYL)IMINO)(METHYLTHIO)METHYL)HYDRAZI  
NYLIDENE)-4-PHENYL-/CN  
E12 1 3-BUTENOIC ACID, 2-(2-((2-PROPEN-1-YLOXY)CARBONYL)OXY)ETHOX  
Y)ETHYL ESTER/CN

```
=> e3
L3      1 "3-BUTENOIC ACID, 2-(2,6-DIMETHYLPHENOXY)-3-METHYL-"/CN

=> file caplus
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
FULL ESTIMATED COST                           ENTRY      SESSION
                                                6.97      7.19
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FILE 'CAPLUS' ENTERED AT 08:03:02 ON 24 FEB 2010  
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FILE COVERS 1907 - 24 Feb 2010 VOL 152 ISS 9  
FILE LAST UPDATED: 23 Feb 2010 (20100223/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> 13
L4      1 L3

=> d 14 ti fbib abs

L4      ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN
TI      p-[(Diethylamino)ethoxy]phenyl-p-tolyl-p-fluorophenylethanol
AN      1963:441367 CAPLUS <>LOGINID:>20100224>>
DN      59:41367
OREF 59:7409c-h
TI      p-[(Diethylamino)ethoxy]phenyl-p-tolyl-p-fluorophenylethanol
AU      Supniewski, J.; Staronkowa, E.
CS      Polish Acad. Sci., Krakow, Pol.
SO      Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences
Biologiques (1962), 10, 185-8
CODEN: BAPBAN; ISSN: 0001-4087
DT      Journal
LA      English
GI      For diagram(s), see printed CA Issue.
AB      1-[p-[(Diethylamino)ethoxy]phenyl]1-(p-tolyl)-2-(p-fluorophenyl)ethanol
(I) prepared as follows, was injected intraperitoneally in 2% solution of the
hydrochloride in daily doses of 50 mg./kg. After 5 days treatment of 10
```

rats, the mean serum cholesterol level fell from  $44.3 \pm 0.7$  to  $23.0 \pm 0.7$  mg.-%. Intraperitoneal injection of I into white mice indicated L.D.50 of 165 mg./kg. The drug induced akinesia, ptosis, and sedation, followed by clonic convulsions and death from respiratory paralysis. For the preparation of I, p-methyl-p-hydroxybenzophenone (II) was prepared by the method of Homer and Medem (CA 47, 1639e). To a mixture of 65 g. II in 26 ml. H<sub>2</sub>O and 250 ml. EtOH containing 24.7 g. NaOH at 10°, 53.3 g. 1-(diethylamino)-2-chloroethane (obtained by heating 1-(diethylamino)-2-hydroxyethane with excess thionyl chloride) was added. The mixture was boiled 1 hr., cooled, the precipitated NaCl removed, and the

EtOH

distilled. The residue (96 g.) in C<sub>6</sub>H<sub>6</sub> was washed with 1% NaOH, and with H<sub>2</sub>O, dried over K<sub>2</sub>CO<sub>3</sub>, and the C<sub>6</sub>H<sub>6</sub> distilled. This residue (93 g.) dissolved in 200 ml. Me<sub>2</sub>CO was added to 250 ml. Me<sub>2</sub>CO containing 38 g. crystalline oxalic acid.

The crude oxalate obtained was washed with Me<sub>2</sub>CO, dried at 105°, and recrystd. from EtOH and Me<sub>2</sub>CO (870:250 ml.) to give 72.3 g. of the oxalate, m. 150-1°. The oxalate in 400 ml. H<sub>2</sub>O was neutralized with 22.5 g. KOH in 35 ml. H<sub>2</sub>O and extracted with C<sub>6</sub>H<sub>6</sub>. The extract dried over K<sub>2</sub>CO<sub>3</sub> and the C<sub>6</sub>H<sub>6</sub> distilled gave 55.3 g.

p-methoxy-p[(diethylamino)ethoxy]benzophenone (III). To 1.15 g. Mg turnings, activated with I in 40 ml. anhydrous Et<sub>2</sub>O, 7.18 g.

p-fluoro-a-chlorotoluene in 50 ml. Et<sub>2</sub>O was added. The mixture was heated 1 hr., cooled, and 10 g. III in 35 ml. Et<sub>2</sub>O added. This mixture was boiled 1 hr., cooled, and poured into 100 ml. H<sub>2</sub>O containing 11 g. NH<sub>4</sub>Cl. The Et<sub>2</sub>O layer was separated and added to the Et<sub>2</sub>O extract of the H<sub>2</sub>O layer. The exts. were washed with H<sub>2</sub>O, dried with Na<sub>2</sub>SO<sub>4</sub>, and the Et<sub>2</sub>O removed. The residue was dissolved in 10 ml. iso-PrOH and 10 ml. ligoine, filtered, and cooled. The separated crystals were washed with iso-PrOH and ligoine (1:1) and dried at 80° to give 79% of I, m. 104-6°. The m.p. was unchanged by recryst. from EtOH and H<sub>2</sub>O.

OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

=> d 14 it

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN  
IT Blood serum  
(cholesterol in, 1-[p-[2-(diethylamino)ethoxy]phenyl]-2-(p-fluorophenyl)-1-p-tolylethanol effect on)  
IT 14753-08-3 93351-45-2  
(Derived from data in the 7th Collective Formula Index (1962-1966))  
IT 90-95-9P, Benzophenone, 4-[2-(diethylamino)ethoxy]-4'-methyl-  
3828-26-0P, Ethanol, 1-[p-[2-(diethylamino)ethoxy]phenyl]-2-(p-fluorophenyl)-1-p-tolyl- 39581-62-9P, Crotonic acid,  
2-(o-hydroxyphenyl)-3-methyl-,  $\gamma$ -lactone 62191-63-3P, Butyric acid, 4-(o-hydroxyphenyl)-3-methyl- 65566-55-4P, Crotonic acid,  
3-methyl-2-phenoxy- 66591-16-0P, 2,5-Cresataldehyde,  
(2,4-dinitrophenyl)hydrazone 75933-69-6P, Crotonic acid, 4-phenoxy-,  
methyl ester 79228-74-3P, Crotonic acid, 3-methyl-4-phenoxy-  
85615-16-3P, 3-Butenoic acid, 4-(o-methoxyphenyl)-3-methyl-, methyl ester  
89641-41-8P, 2-Pentenoic acid, 2-bromo-, methyl ester 90843-51-9P,  
Crotonic acid, 2-phenoxy- 91142-96-0P, 3-Butenoic acid,  
4-(o-hydroxyphenyl)-3-methyl-, 91496-48-9P, 3-Butenoic acid,  
4-(o-hydroxyphenyl)-3-methyl-, methyl ester 91496-59-2P, Crotonic acid,  
3-methyl-2-phenoxy-, methyl ester 91496-60-5P, Crotonic acid,  
3-methyl-4-phenoxy-, methyl ester 91496-61-6P, Crotonic acid,  
3-methyl-2-(p-tolyl)- 91496-62-7P, Crotonic acid,  
3-methyl-4-(p-tolyl)- 91496-90-1P, 3-Pentenoic acid,  
4-(o-hydroxyphenyl)-, methyl ester 92016-85-8P, 3-Butenoic acid,  
3-methyl-4-phenoxy- 92016-89-2P, Crotonic acid, 2-phenoxy-, methyl ester

92016-98-3P, 2-Pentenoic acid, 2-phenoxy- 92864-20-5P, 3-Butenoic acid,  
 3-methyl-2-(2,6-xylyloxy)-, methyl ester 92864-34-1P, Crotonic acid,  
 3-methyl-2-(2,6-xylyloxy)-, methyl ester 92864-35-2P, Crotonic acid,  
 3-methyl-4-(2,6-xylyloxy)-, methyl ester 93305-47-6P, Crotonic acid,  
 2-(6-hydroxy-m-tolyl)-3-methyl-,  $\gamma$ -lactone 93351-67-8P, Valeric  
 acid, 4-(o-hydroxyphenyl)- 97024-30-1P, Crotonic acid,  
 3-methyl-2-(p-tolylloxy)-, methyl ester 97024-31-2P, Crotonic acid,  
 3-methyl-4-(p-tolylloxy)-, methyl ester 97024-32-3P, Crotonic acid,  
 3-methyl-2-(2,6-xylyloxy)- 98017-53-9P, 3-Butenoic acid,  
 4-(6-hydroxy-m-tolyl)-3-methyl-, methyl ester 98017-54-0P,  
 3-Butenoic acid, 3-methyl-2-(2,6-xylyloxy)- 98017-58-4P, Crotonic acid,  
 3-methyl-4-(2,6-xylyloxy)- 106404-90-4P, Benzophenone,  
 4-[2-(diethylamino)ethoxy]-4'-methyl-, oxalate 859038-83-8P, Butyric  
 acid, 4-(6-hydroxy-m-tolyl)-3-methyl-  
 RL: PREP (Preparation)  
 (preparation of)

=> 98017-54-0

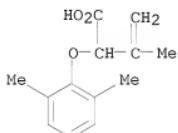
REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
 Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L6 1 L5

=> display hitstr 16  
 ENTER ANSWER NUMBER OR RANGE (1):1

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN  
 IT 98017-54-0P, 3-Butenoic acid, 3-methyl-2-(2,6-xylyloxy)-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 98017-54-0 CAPLUS  
 CN 3-Butenoic acid, 2-(2,6-dimethylphenoxy)-3-methyl- (CA INDEX NAME)



=> file reg  
 COST IN U.S. DOLLARS  
 FULL ESTIMATED COST

| SINCE FILE<br>ENTRY | TOTAL<br>SESSION |
|---------------------|------------------|
| 7.52                | 20.19            |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE                        | 0.00             | -0.85         |

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STRUCTURE FILE UPDATES: 22 FEB 2010 HIGHEST RN 1207159-36-1  
DICTIONARY FILE UPDATES: 22 FEB 2010 HIGHEST RN 1207159-36-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d his

(FILE 'HOME' ENTERED AT 08:00:54 ON 24 FEB 2010)

FILE 'REGISTRY' ENTERED AT 08:01:10 ON 24 FEB 2010  
STRUCTURE uploaded  
L1 2 SEARCH L1 SSS SAM  
L2 E 3-BUTENOIC ACID, 2-(2,6-DIMETHYLPHENOXY)-3-METHYL-/CN  
L3 1 E3

FILE 'CAPLUS' ENTERED AT 08:03:02 ON 24 FEB 2010  
L4 1 L3  
S 98017-54-0/REG#

FILE 'REGISTRY' ENTERED AT 08:04:38 ON 24 FEB 2010  
L5 1 S 98017-54-0/RN

FILE 'CAPLUS' ENTERED AT 08:04:39 ON 24 FEB 2010  
L6 1 S L5

FILE 'REGISTRY' ENTERED AT 08:07:36 ON 24 FEB 2010

=> search l1 sss full  
FULL SEARCH INITIATED 08:09:08 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 30069 TO ITERATE

100.0% PROCESSED 30069 ITERATIONS 28 ANSWERS  
SEARCH TIME: 00.00.01

L7 28 SEA SSS FUL L1

=> d scan

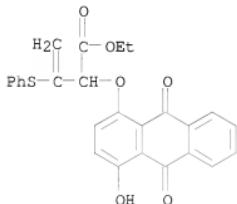
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Hexenoic acid, 3-methyl-5-oxo-2-phenoxy-  
MF C13 H14 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):38

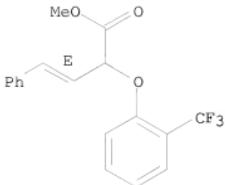
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-[(9,10-dihydro-4-hydroxy-9,10-dioxo-1-anthracyanyl)oxy]-  
3-(phenylthio)-, ethyl ester  
MF C26 H20 O6 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 4-phenyl-2-[2-(trifluoromethyl)phenoxy]-, methyl ester,  
(3E)-  
MF C18 H15 F3 O3

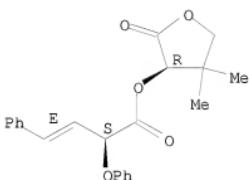
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

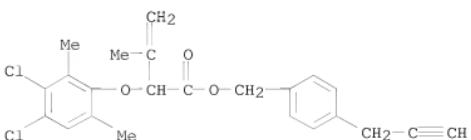
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-phenoxy-4-phenyl-,  
(3R)-tetrahydro-4,4-dimethyl-1-oxo-3-furanyl ester, (2S,3E)-  
MF C22 H22 O5

Absolute stereochemistry.  
Double bond geometry as shown.



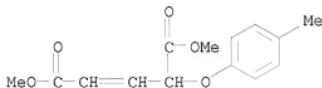
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-(3,4-dichloro-2,6-dimethylphenoxy)-3-methyl-,  
[4-(2-propynyl-1-yl)phenyl]methyl ester  
MF C23 H22 Cl2 O3



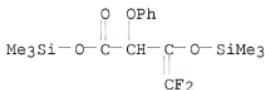
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN INDEX NAME NOT YET ASSIGNED  
MF C14 H16 O5



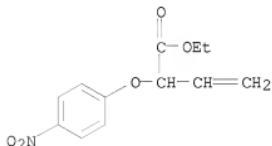
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 4,4-difluoro-2-phenoxy-3-[(trimethylsilyl)oxy]-,  
trimethylsilyl ester  
MF C16 H24 F2 O4 Si2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

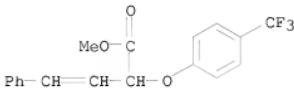
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-(4-nitrophenoxy)-, ethyl ester  
MF C12 H13 N O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

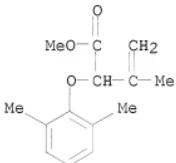
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 3-Butenoic acid, 4-phenyl-2-[4-(trifluoromethyl)phenoxy]-, methyl ester  
MF C18 H15 F3 O3



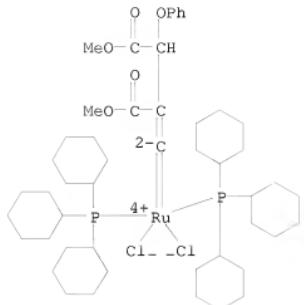
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-(2,6-dimethylphenoxy)-3-methyl-, methyl ester  
MF C14 H18 O3



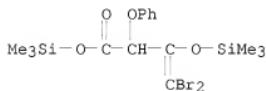
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN Ruthenium, dichloro[4-methoxy-2-(methoxycarbonyl)-4-oxo-3-phenoxy-1-buten-1-ylidene]bis(tricyclohexylphosphine)-, (SP-5-31)-  
MF C49 H78 Cl2 O5 P2 Ru  
CI CCS



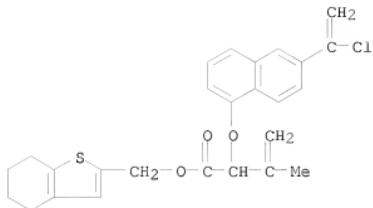
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 4,4-dibromo-2-phenoxy-3-((trimethylsilyl)oxy)-, trimethylsilyl ester  
 MF C16 H24 Br2 O4 Si2



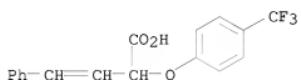
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-[(6-(1-chloroethenyl)-1-naphthalenyl)oxy]-3-methyl-, (4,5,6,7-tetrahydrobenzo[b]thien-2-yl)methyl ester  
 MF C26 H25 Cl O3 S



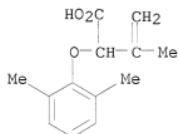
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 4-phenyl-2-[4-(trifluoromethyl)phenoxy]-  
 MF C17 H13 F3 O3



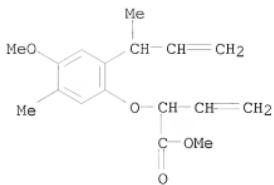
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-(2,6-dimethylphenoxy)-3-methyl-  
 MF C13 H16 O3



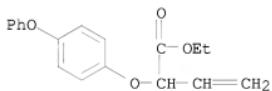
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-[4-methoxy-5-methyl-2-(1-methyl-2-propen-1-yl)phenoxy]-  
 , methyl ester  
 MF C17 H22 O4



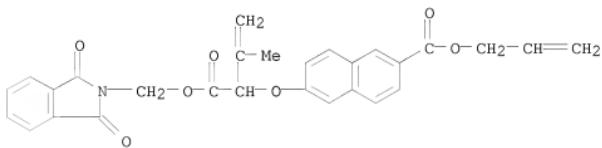
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-(4-phenoxyphenoxy)-, ethyl ester  
 MF C18 H18 O4



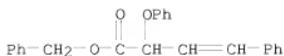
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 2-Naphthalene carboxylic acid, 6-[[1-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methoxy]carbonyl]-2-methyl-2-propenyl]oxy]-, 2-propenyl ester  
 MF C28 H23 N O7



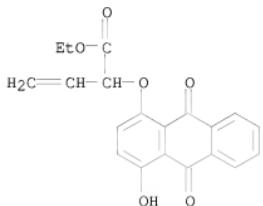
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-phenoxy-4-phenyl-, phenylmethyl ester  
 MF C23 H20 O3



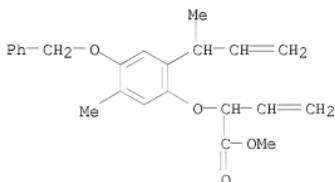
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-[(9,10-dihydro-4-hydroxy-9,10-dioxo-1-anthracenyl)oxy]-  
 , ethyl ester  
 MF C20 H16 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

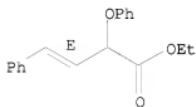
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-[5-methyl-2-(1-methyl-2-propen-1-yl)-4-  
 (phenylmethoxy)phenoxy]-, methyl ester  
 MF C23 H26 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

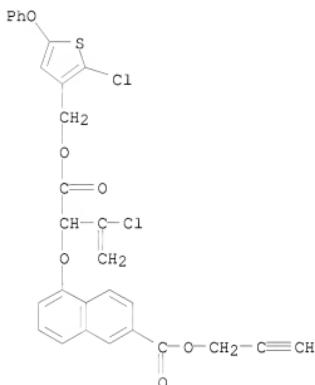
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-phenoxy-4-phenyl-, ethyl ester, (E)- (9CI)  
MF C18 H18 O3

Double bond geometry as shown.



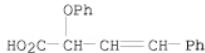
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 2-Naphthalene carboxylic acid, 5-[[2-chloro-1-[(2-chloro-5-phenoxy-3-thienyl)methoxy]carbonyl]-2-propen-1-yl]oxy-, 2-propyn-1-yl ester  
MF C29 H20 Cl2 O6 S



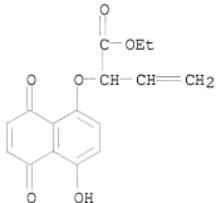
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-phenoxy-4-phenyl-  
MF C16 H14 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

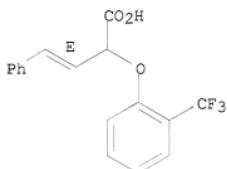
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-[(5,8-dihydro-4-hydroxy-5,8-dioxo-1-naphthalenyl)oxy]-, ethyl ester  
MF C16 H14 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

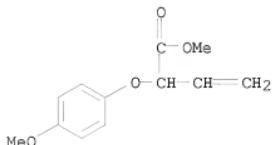
L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 4-phenyl-2-[2-(trifluoromethyl)phenoxy]-, (3E)-  
MF C17 H13 F3 O3

Double bond geometry as shown.



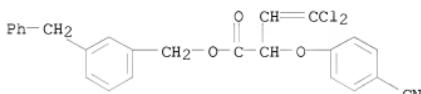
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 2-(4-methoxyphenoxy)-, methyl ester  
MF C12 H14 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 28 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 3-Butenoic acid, 4,4-dichloro-2-(4-cyanophenoxy)-,  
[3-(phenylmethyl)phenyl]methyl ester  
MF C25 H19 C12 N O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

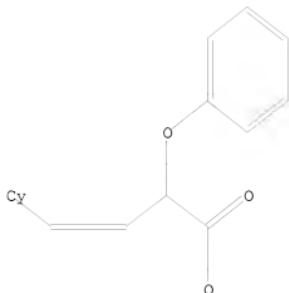
ALL ANSWERS HAVE BEEN SCANNED

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files\10566995\10566995 two-ring cmpds.str

L8 STRUCTURE UPLOADED

=> d 18  
L8 HAS NO ANSWERS  
L8 STR



Structure attributes must be viewed using STN Express query preparation.

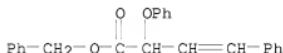
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 FULL SUBSET SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 8 ANSWERS  
 SEARCH TIME: 00.00.01

L9 8 SEA SUB=L7 SSS FUL L8

=> d scan

L9 8 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-phenoxy-4-phenyl-, phenylmethyl ester  
 MF C23 H20 O3

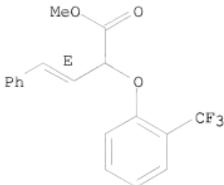


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

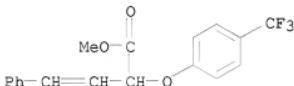
L9 8 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 4-phenyl-2-[2-(trifluoromethyl)phenoxy]-, methyl ester,  
 (3E)-  
 MF C18 H15 F3 O3

Double bond geometry as shown.



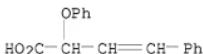
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 8 ANSWERS  REGISTRY  COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 4-phenyl-2-[4-(trifluoromethyl)phenoxy]-, methyl ester  
 MF C18 H15 F3 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

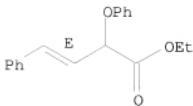
L9 8 ANSWERS  REGISTRY  COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-phenoxy-4-phenyl-  
 MF C16 H14 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

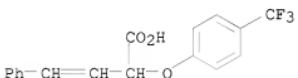
L9 8 ANSWERS  REGISTRY  COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-phenoxy-4-phenyl-, ethyl ester, (E)- (9CI)  
 MF C18 H18 O3

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

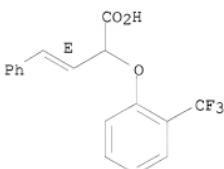
L9 8 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 4-phenyl-2-[4-(trifluoromethyl)phenoxy]-  
 MF C17 H13 F3 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 8 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 4-phenyl-2-[2-(trifluoromethyl)phenoxy]-, (3E)-  
 MF C17 H13 F3 O3

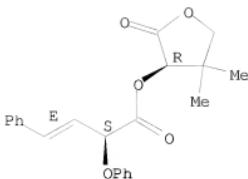
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L9 8 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN 3-Butenoic acid, 2-phenoxy-4-phenyl-,  
 (3R)-tetrahydro-4,4-dimethyl-2-oxo-3-furanyl ester, (2S,3E)-  
 MF C22 H22 O5

Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

|  |            |         |  |
|--|------------|---------|--|
| => file caplus                             |            |         |  |
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|  | ENTRY      | SESSION |  |
| FULL ESTIMATED COST                        | 242.92     | 263.11  |  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |  |
|  | ENTRY      | SESSION |  |
| CA SUBSCRIBER PRICE                        | 0.00       | -0.85   |  |

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 FILE LAST UPDATED: 23 Feb 2010 (20100223/ED)  
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009  
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 19

L10 4 L9

=> d 110 1-4 ti fbib abs

L10 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN  
TI Preparation of 4-phenyl-but-3-enoic acid derivatives, as peroxisome  
proliferator-activated receptors (PPAR) ligands, in particular PPAR $\alpha$   
and PPAR $\gamma$  agonists, for the treatment and prevention of diabetes,  
dyslipidemia, atherosclerosis  
AN 2005:119915 CAPLUS <>LOGINID:20100224>  
DN 142:219047  
TI Preparation of 4-phenyl-but-3-enoic acid derivatives, as peroxisome  
proliferator-activated receptors (PPAR) ligands, in particular PPAR $\alpha$   
and PPAR $\gamma$  agonists, for the treatment and prevention of diabetes,  
dyslipidemia, atherosclerosis  
IN Zeiller, Jean Jacques; Dumas, Herve; Guyard Dangremont, Valerie; Berard,  
Isabelle; Contard, Francis; Guerrier, Daniel; Ferrand, Gerard; Bonhomme,  
Yves  
PA Merck Sante, Fr.  
SO Fr. Demande, 38 pp.  
CODEN: FRXXBL  
DT Patent  
LA French  
FAN.CNT 1

|     | PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE       |
|-----|---|------|----------|-----------------|------------|
| PI  | FR 2858615  | A1   | 20050211 | FR 2003-9610    | 20030804   |
|     | FR 2858615  | B1   | 20061222 | FR 2003-9610    | A 20030804 |
|     | AU 2004263254   | A1   | 20050217 | AU 2004-263254  | 20040714   |
|     |   |      |          | FR 2003-9610    | W 20040714 |
|     |   |      |          | WO 2004-EP7776  | W 20040714 |
| CA  | 2534493   | A1   | 20050217 | CA 2004-2534493 | 20040714   |
|     |   |      |          | FR 2003-9610    | A 20030804 |
|     |   |      |          | WO 2004-EP7776  | W 20040714 |
| WO  | 2005014521  | A1   | 20050217 | WO 2004-EP7776  | 20040714   |
| W:  | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,<br>CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,<br>GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,<br>LK, LR, LS, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,<br>NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,<br>TJ, TM, TN, TR, TT, TZ, UA, US, UZ, VC, VN, YU, ZA, ZM, ZW |      |          |                 |            |
| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,<br>AM,<br>AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,<br>EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,<br>SI, SK, TR, BF, BJ, CF, CG, CI, GM, GA, GN, GQ, GW, ML, MR, NE,<br>SN, TD, TG   |      |          |                 |            |
| EP  | 1658260   | A1   | 20060524 | FR 2003-9610    | A 20030804 |
|     |   |      |          | EP 2004-740992  | 20040714   |
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|     |   |      |          | FR 2003-9610    | A 20030804 |
|     |   |      |          | WO 2004-EP7776  | W 20040714 |
| JP  | 2007501190  | T    | 20070125 | JP 2006-522255  | 20040714   |
|     |   |      |          | FR 2003-9610    | A 20030804 |
|     |   |      |          | WO 2004-EP7776  | W 20040714 |
| US  | 20060178434   | A1   | 20060810 | US 2006-566995  | 20060202   |
|     |   |      |          | FR 2003-9610    | A 20030804 |
|     |   |      |          | WO 2004-EP7776  | W 20040714 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS CASREACT 142:219047; MARPAT 142:219047

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [wherein R1 = alkyl, (un)substituted heterocycl, (un)substituted aryl or/and (un)condensed with a (un)saturated monocyclic or polycyclic; R2, R3 = independently H, (un)substituted aryl; or R2R3 = alkylene; R = H, aryl/alkyl; their acid and base addition salts; with proviso; their derivs., solvates, and stereoisomers and their mixts., and their pharmaceutically acceptable salts] were prepared as peroxisome proliferator-activated receptors (PPAR)- $\alpha$  and PPAR $\gamma$  agonists for treating diabetes, dyslipidemia, atherosclerosis (no data). For example, II was prepared, in 4 steps, reacting 2-oxo-4-phenylbut-3-enoic acid sodium salt with methanol, followed by reduction, alkylation of the alc. with MeI, and saponification III at a concentration of 50  $\mu$ M was a PPAR $\alpha$  and PPAR $\gamma$  agonist, showing induced luciferase activity via PPAR $\alpha$ /Gal4 and PPAR $\gamma$ /Gal4 with a factor of induction of 2.3 and 6.4, resp. Thus, I and their compns. are useful for treating and preventing dyslipidemia, atherosclerosis and diabetes (no data).

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN  
TI Chiral catalyst enhancement of diastereocontrol for O-H insertion reactions of styryl- and phenyldiazoacetate esters of pantolactone  
AN 2002:586128 CAPLUS <LOGINID:20100224>  
DN 138:89461  
TI Chiral catalyst enhancement of diastereocontrol for O-H insertion reactions of styryl- and phenyldiazoacetate esters of pantolactone  
AU Doyle, Michael P.; Yan, Ming  
CS Department of Chemistry, University of Arizona, Tucson, AZ, 85721-0041, USA  
SO Tetrahedron Letters (2002), 43(34), 5929-5931  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
OS CASREACT 138:89461  
AB The chiral dirhodium(II) catalyst Rh<sub>2</sub>(MEAZ) <sub>4</sub> (Me 4-oxo-2-azetidinecarboxylate) increases diastereocontrol for intermol. O-H insertion reactions of diazo esters having a chiral auxiliary over that achieved with Rh<sub>2</sub>(OAc)<sub>4</sub>.  
OSC.G 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS RECORD (29 CITINGS)  
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN  
TI A Stereoselective Access to Allylic Systems Using Rhodium(II)-Vinyl Carbenoid Insertion into Si-H, O-H, and N-H Bonds  
AN 1997:198048 CAPLUS <LOGINID:20100224>  
DN 126:211638  
OREF 126:40925a, 40926a  
TI A Stereoselective Access to Allylic Systems Using Rhodium(II)-Vinyl Carbenoid Insertion into Si-H, O-H, and N-H Bonds  
AU Bulugahapitiya, Priyadarshanie; Landais, Yannick; Parra-Rapado, Liliana; Planchenault, Denis; Weber, Valery  
CS College Propedeutique, Universite de Lausanne, Lausanne-Dorigny, 1015, Switz.

SO Journal of Organic Chemistry (1997), 62(6), 1630-1641

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

AB Rhodium-catalyzed decomposition of  $\alpha$ -vinyl diazo esters in the presence of silanes, alcs., ethers, amines, and thiols has been shown to produce the corresponding  $\alpha$ -silyl,  $\alpha$ -hydroxy,  $\alpha$ -alkoxy,  $\alpha$ -amino, and  $\alpha$ -thioalkoxy esters in generally good yield with a complete retention of the stereochem. of the double bond of the diazo precursor. An extension of the process in homochiral series has also been devised using either a chiral auxiliary attached to the ester function or achiral  $\alpha$ -vinyl diazo esters and Doyle's chiral catalyst Rh2(MEPY)4. In the former approach, pantolactone as chiral auxiliary gave diastereoselectivities of up to 70%, while the second approach produced the desired allylsilane with ee as high as 72%. On the other hand, Rh2(MEPY)4-catalyzed insertion into the O-H bond of water led to poor or no enantioselectivity in good agreement with recent literature reports.

OSC.G 58 THERE ARE 58 CAPLUS RECORDS THAT CITE THIS RECORD (59 CITINGS)

RE.CNT 119 THERE ARE 119 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

TI Electronic versus steric effects in 5-endo-trig-like electrophilic cyclizations

AN 1995:974892 CAPLUS <<LOGINID::20100224>>

DN 124:176328

OREF 124:32707a,32710a

TI Electronic versus steric effects in 5-endo-trig-like electrophilic cyclizations

AU Landais, Yannick; Planchenault, Denis

CS Inst. de Chimie Organique, Univ. de Lausanne, Lausanne-Dorigny, 1015, Switz.

SO Synlett (1995), (11), 1191-3

CODEN: SYNLES; ISSN: 0936-5214

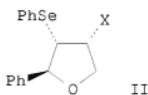
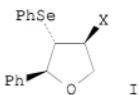
PB Thieme

DT Journal

LA English

OS CASREACT 124:176328

GI



AB Electronically and sterically differentiated allylic substituents such as RO, NHPh, PhS, and PhSO2 groups were used to demonstrate the influence of electronic and/or steric effects in the stereocontrol of the PhSeCl-promoted electrophilic 5-endo-trig-like cyclizations of 2-substituted-3-alkenols, (E)-PhCH:CHCHXCH2OH (1, X = OH, OEt, OCH2CF3, OPh, NHPh, SPh). 1 Reacted with PhSeCl/K2CO3 to give predominantly the 2,4-trans-tetrahydrofuran I, however, the cis-2,4-diastereoisomer II was predominant for X = NHPh and SPh for reasons of electronic effects.

OSC.G 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

=>  
=> logoff hold  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST  
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  
CA SUBSCRIBER PRICE

|  | SINCE FILE | TOTAL   |
|--|------------|---------|
|  | ENTRY      | SESSION |
| FULL ESTIMATED COST                        | 25.90      | 289.01  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
| CA SUBSCRIBER PRICE                        | ENTRY      | SESSION |
|  | -3.40      |         |